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FINAL REPORT ON OFFICE OF NAVAL RESEARCH CONTRACT

N 00014-79-C-0766, RF4119

"ION-ATOM COLLISIONS"

Prepared by

J. F. Reading and A. L. Ford

Department of Physics, Texas A&M University,

College station, Texas 77843

SUMMARY

Theoretical studies of ion-atom collisions in the intermediate energy range have been carried out. Detailed comparisions to experimental measurements of the inner shell processes of ionization and charge transfer have been made. They confirm the reliability of our ab initio theoretical approach to these previously unsolved problems.

We have concentrated on three areas.

a) Light ion projectiles where probabilities for all except elastic processes are small.

b) Somewhat heavier projectiles such as fully stripped lithium and carbon. Here the full richness of the many electron target comes into play, through interference among the various processes.

c) Symmetric situations where the charges of the projectile and the target nuclei are comparable. Here in the velocity matching region charge transfer plays an important role for electron flux loss from the target.

The advantage of a reliable theoretical method is that meaningful conclusions can now be drawn from experiments. We have for example built a considerable case for a previously unconsidered physical process being important in charge transfer i.e. "knock-off" of the captured electron by the outer shells of the target. We have also demonstrated that multi electron processes can play a dramatic role in "two state" processes such as charge transfer accompanied by hole production. This particular phenomena is unique to atomic physics and demonstrates that purely quantum phenomena can change total cross sections by factor of two or three. This certainly casts doubt on the reliability of the classical

method for collisions of many body systems.

These two new results follow from comparison of good theory and experiment. But in the symmetric region no theoretical method was available that was both practically and mathematically adequate. A new theoretical approach called a one and a half centered expansion (OHCE) has been developed by us and successfully tested in the proton-hydrogen system. We feel that the OHCE will play a major role in this field in the next decade.

Other areas of investigation, not completed, but on which considerable progress has been made, are collisions with negatively charged projectiles, impact parameter dependence studies of charge transfer and L- shell ionization.

We are also pleased to report that this contract has allowed us to travel and disemiminate the progress we have made so our methods have become generally known. In particular the Naval Surface Weapons Center at Silver Springs is now using our codes on its research.

INTRODUCTION

Ion-atom collisions in the intermediate energy region are of great practical interest to many branches of physics. If absolute X-ray cross sections are known in situ quantitative analysis of elements is possible. Thus wear on gun barrels can be accurately measured, or hair types analyzed for forensic investigations. Stopping powers are of tremendous importance to the design of reactors or ion beams used to intercept missiles, charge transfer is important in fusion and astrophysics.

Spurred by recent experimental efforts in this area our group has developed a research program with the aim of producing and using computer codes which can calculate cross sections for ion-atom collisions. This report describes the progress we have made in the last year with money provided by ONR.

Our aim has been to design methods which are applicable to the actual situation encountered in a genuine ion atom collision. For example, as an accurate description of an electron moving in the field of an atom involves numerical non local potentials. Thus we discard at the outset all schemes, such as the Glauber approximation, which need simple analytical forms to be affected. Secondly, we regard as an essential feature of any method we develope that its accuracy should be simply determinable. For example by increasing the number of basis states in our calculation we can get a very good idea of the errors. But we reject classical methods, first or second order Born theories, impulse or distorted wave approximations and so on, as generally it is not easy to implement a program of systematic improvement in the accuracy of such approaches. However these approximation schemes

are very efficient in the use of computor time. Of course computational efficiency is an essential feature of a good method. We have paid great attention to this. But even with modern computers it is very easy to exceed the capabilities of any machine in a many body system collision. And lastly of course luck rather than forsight has played an important role in our research. We had developed computational methods specifically using the fact that charge transfer was not important in the a-symmetric region. By asymmetric we mean systems in which the projectile charge Z_p is much less than the target nuclear charge Z_n. It was completely unknown to us as little as six months ago that a trivial conversion of this asymmetric code could extend its applicability into the symmetric region with the same computational efficiency. This new method, called a one and a half centered expansion (OHCE) method, will play a vital role in our work in the next decade.

In the next section we summarize the results of three in depth investigations we have carried out. In section III we describe our ongoing program.

II. (a) Inner-shell capture in collisions of H^+ projectiles with Neon, Carbon, and Argon.

Here we have used a trial wave function

$$\psi_1(SCE) = \sum_{n=1}^{N} c_{n1}(t)\,\chi_n(\vec{r},t) \qquad (1)$$

where the set $\{\chi_n\}$ are target centered pseudostates, angular momentum ℓ = 0, 1 and 2, eigenstates to the Hartree-Fock target Hamiltonian H_T, projected onto a hilbert basis.

As charge transfer is an unimportant channel for electron flux loss from the target, it is not included explicitly in the trial wave function. For this reason we refer to eq(1) as being a single centered expansion (SCE) method. Charge transfer amplitudes $b_{m1}(\infty)$ are calculated from the t-matrix integral

$$b_{m1}(\infty) = \frac{-i}{\hbar}\int_{-\infty}^{\infty} dt \,\langle \phi_m(\vec{r},t)|V_T|\psi_1(SCE)\rangle, \qquad (2).$$

where ϕ_m are eigenstates on the moving projectile and V_T is the single electron target potential. The coefficients $c_{n1}(t)$ are found by imposing the variational conditions that

$$\langle \chi_n(\vec{r},t)|\, i\hbar\frac{\partial}{\partial t} - H_T - V_p\, |\psi_1(SCE)\rangle = 0, \qquad (3)$$

where V_p is the perturbation provided by the projectile following a classical coulombic trajectory.

We calculate charge transfer accompanied by hole production in the K shell. Our calculations for hydrogen ions (protons) on carbon, neon and argon targets are given in fig. 1-3, where comparison is made to the experiments of Rodbro et al (Phys. Rev. A19, 1936 (1979)) and to the earlier experiments of Cocke et al. (Phys. Rev. A16, 7748 (1977)).

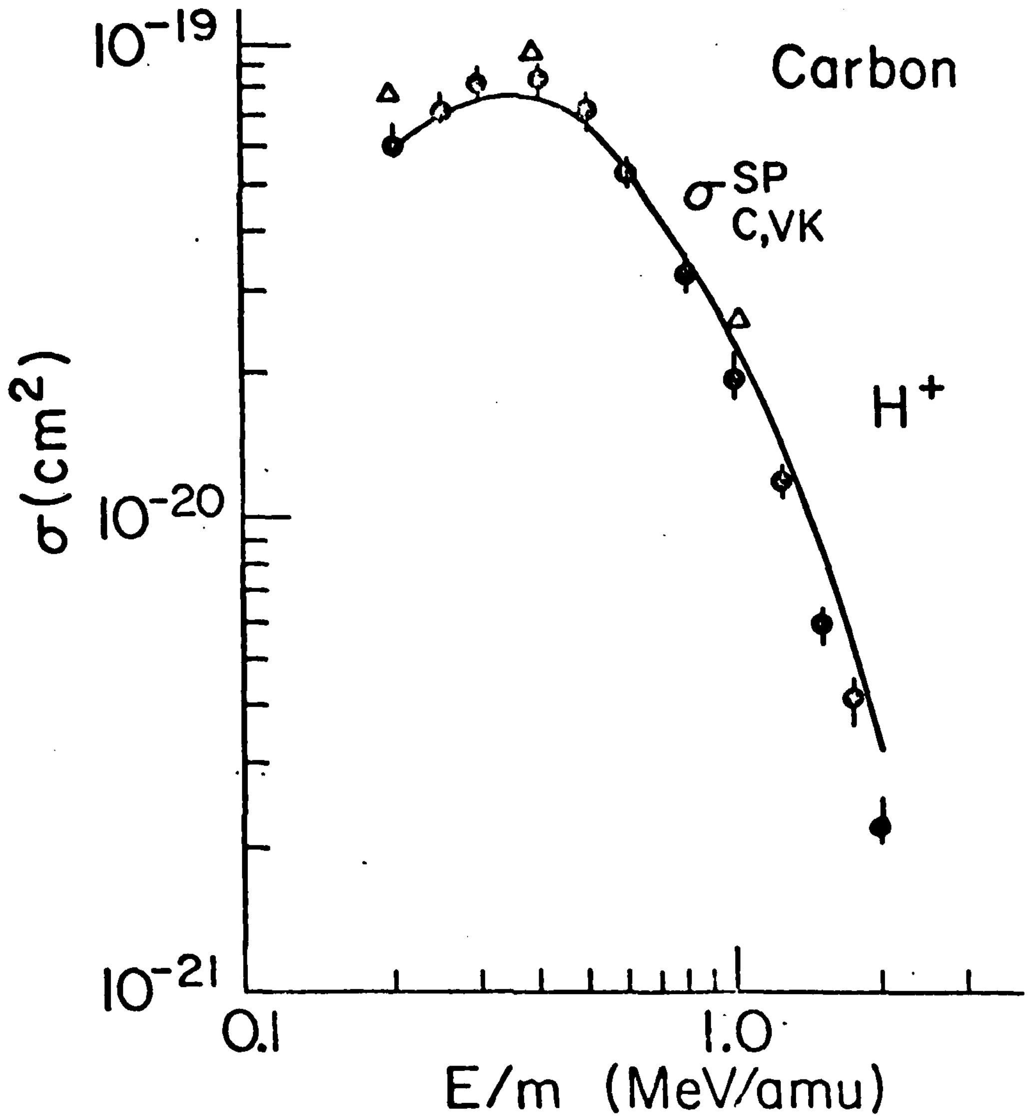


Fig. 1. Cross sections $\sigma_{C,VK}$ for a hydrogen ion producing the charge transfer state in coincidence with a K shell hole in the Carbon target. Theory, solid curve. Experiment, circles, from Rodbro et al.

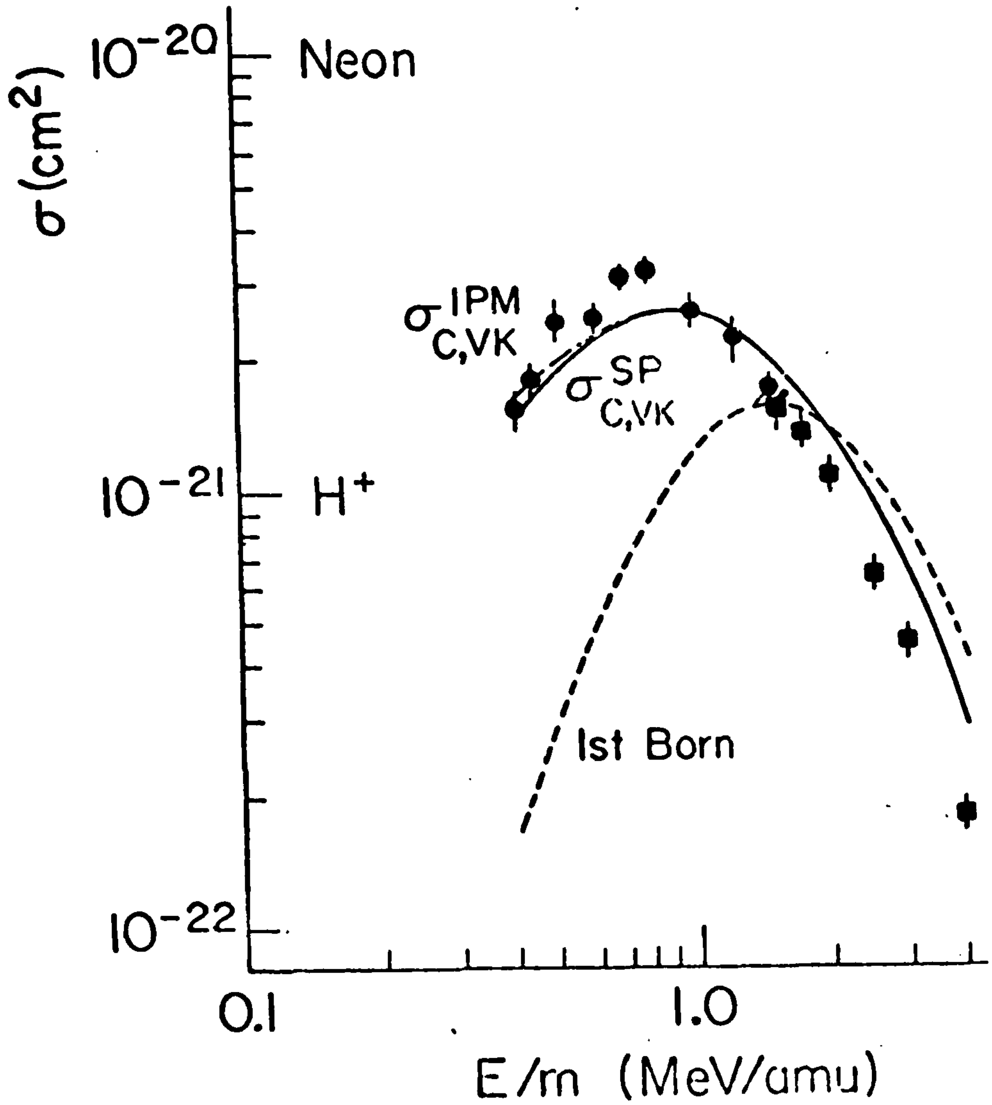


Fig. 2. Cross sections $\sigma_{C,VK}$ for a hydrogen ion producing the charge transfer state in coincidence with a K-shell hole in Neon. Theory, solid curve. The dashed curve represents a first Born calculation. Experiments are from Cocke et al, squares, and Rodbro et al, circles.

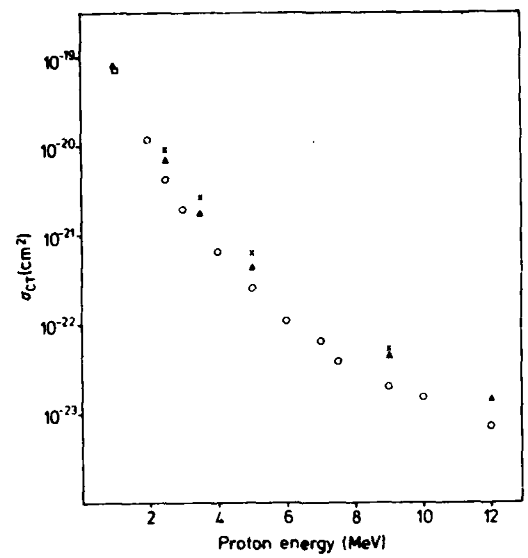


Fig. 3. Total charge capture cross sections for hydrogen ions incident on argon. The triangles are our results with s, p, and d partial waves; the crosses are our results if ony s and p partial waves are used in the calculation. Experiments from Rodbro et al, open square, and Macdonald et al, Phys. Rev. Lett, 37, 648 (1974), open circles.

As can be seen from figs. 1 through 3 reasonable agreement is obtained between theory and experiment. However there is a definite tendency for the theory to lie above experiment as the number of electrons in the outer shell of the target atom increases. A possible explanation for this is "knock off" of the captured electron in inelastic collision with the outer shells. Experiments with higher Z_n targets could confirm this.

(b). He^{2+}, Li^{3+} and C^{4+} and C^{6+} direct ionization and charge transfer on various targets.

As the charge of the projectile is increased charge transfer itself plays an increasingly important part in K-shell hole production. The cross section for the charge transfer part of this reaction may be inferred from two experiments: one where the projectile K-shell is empty, C^{6+}, and another where it is full. In fig. 4 we show a comparison of theory and experiment for this process. Note this confirms the ability of our code to simultaneously calculate K-shell direct ionization, the C^{4+} result, and charge transfer, the difference between the two results.

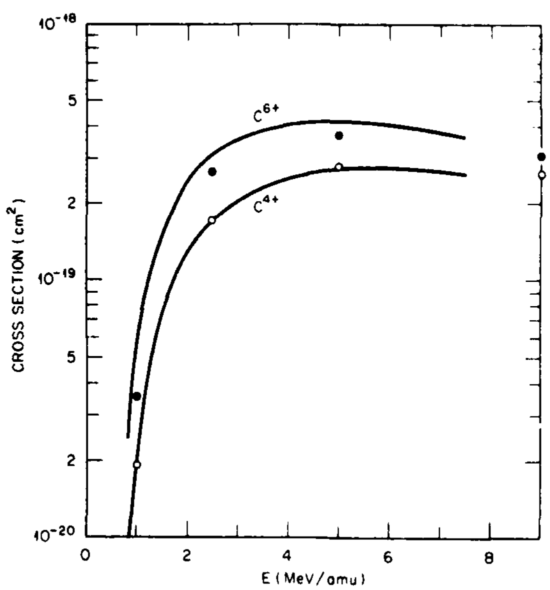


Fig. 4. Theoretical cross sections for K-shell vacancy production in Ar by C^{6+} (full circles) and C^{4+} (open circles) projectiles. The solid curve experimental results are the smooth curves through data presented by Tawara et al Phys. Rev. Lett, 59a, 14, (1976).

As the charge of the projectile increases the probability for simultaneous interaction of the projectile with two or more electrons is of the same order as a single electron interaction probability. In these circumstances the identity of the electrons plays a crucial role as discussed by the present authors (Phys. Rev. A21, 124 (1980)).

An example of this is given in fig. 5 for He^{2+} and Li^{3+} projectiles on Neon.

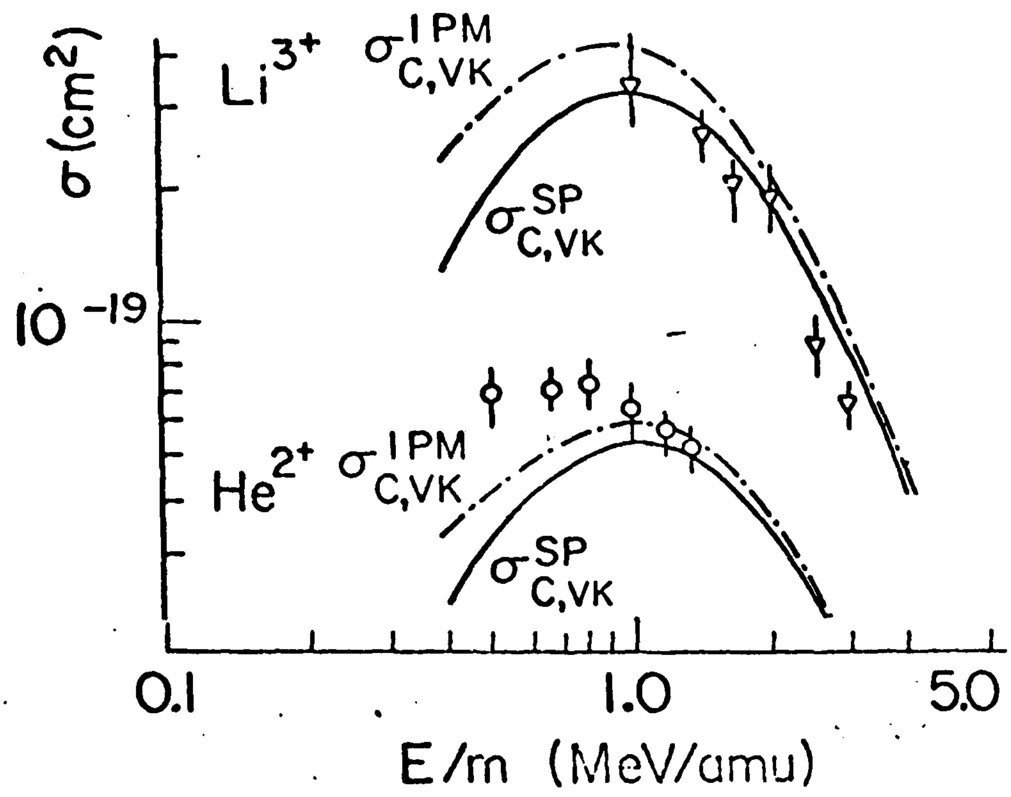


Fig. 5. The actual cross section for a vacancy produced in the K-shell accompanied by charge transfer to the projectile, $\sigma^{IPM}_{C,VK}$ and that cross section that would obtain if the only Neon Target electrons were the two K-shell electrons, $\sigma^{SP}_{C,VK}$

The difference between the curves is caused by multielectron interference between the amplitudes for different electrons of the same spin undergoing simultaneous transition. The experimental cross section is $\sigma^{IPM}_{c,VK}$.

The other cross section $\sigma^{SP}_{c,VK}$, the single particle prediction, can be inferred from an experiment as in Fig. 4. The quantum mechanical interference effect cannot be reproduced from classical calculations.

(c) The Symmetric Region

As the charge of the projectile is increased charge transfer becomes an important mechanism for electron loss from the target. It must therefore be somehow incorporated in the trial wave function ansatz. A conventional way to solve this problem is a two centered expansion method (TCE).

$$\psi_1(\mathrm{TCE}) = \sum_{n=1}^{N} a_{n1}(t)\,\chi_n(\vec{r},t) + \sum_{m=1}^{M} b_{m1}(t)\,\phi_m(\vec{r},t). \qquad (4)$$

Unfortunately this leads to a set of coupled differential equations, which as the sets $\{\chi_n\}$ and $\{\phi_m\}$ are not mutually orthogonal, must be diagonalized at each step. Hence this method is very expensive in its use of computer time. Further, as the basis is increased to include enough states to properly describe the multielectron interference effects discussed above, and to properly span the energy spectrum of ejected electrons, the sets $\{\chi_n\}$ and $\{\phi_m\}$ become linearly dependent. The equations for a_{n1} and b_{m1} become ill conditioned.

A way out of this is to use a one and a half centered expension, (OHCE).

$$\psi_1(\mathrm{OHCE}) = \sum_{n=1}^{N} a_{n1}(t)\,\chi_n(\vec{r},t) + \sum_{m=1}^{M} b_{m1}(\infty)\,\phi_m(\vec{r},t)\,\beta_m(t) \qquad (5)$$

Here $\beta_m(t)$ is a prechosen function of time subject only to the boundary conditions that $\beta_m(-\infty)=0$, $\beta_m(\infty)=1$.

The coefficients $a_{n1}(t)$ are found by applying the condition of eq. (3). The charge transfer amplitudes are found by applying one of two alternative constraints.

$$\int_{-\infty}^{+\infty} \langle \phi_m(\vec{r},t) | i\hbar \frac{\partial}{\partial t} - H_T - V_P | \psi_1(\mathrm{OHCE}) \rangle dt = 0, \tag{6a}$$

or

$$\int_{-\infty}^{+\infty} \beta_m(t) \langle \phi_m(\vec{r},t) | i\hbar \frac{\partial}{\partial t} - H_T \; V_P | \psi_1(\mathrm{OHCE}) \rangle dt = 0. \tag{6b}$$

The former constraint is equivalent to eq (2) and we call it a perturbative choice. The latter constraint leads to the condition that

$$\sum_{n=1}^{N} |a_{n1}(\infty)|^2 + \sum_{m=1}^{M} |b_{m1}(\infty)|^2 = 1,$$

and hence is called a unitary constraint. In figs. 6-8 we show the failure of the SCE method or the proton-hydrogen system. It fails because the trial wave function cannot adequately describe the flux loss due to charge transfer in the velocity matching region (30keV). But the new method corrects this deficiency and produces very good agreement with the experiment in a calculation remarkable in its computational efficiency.

III. Work in Progress

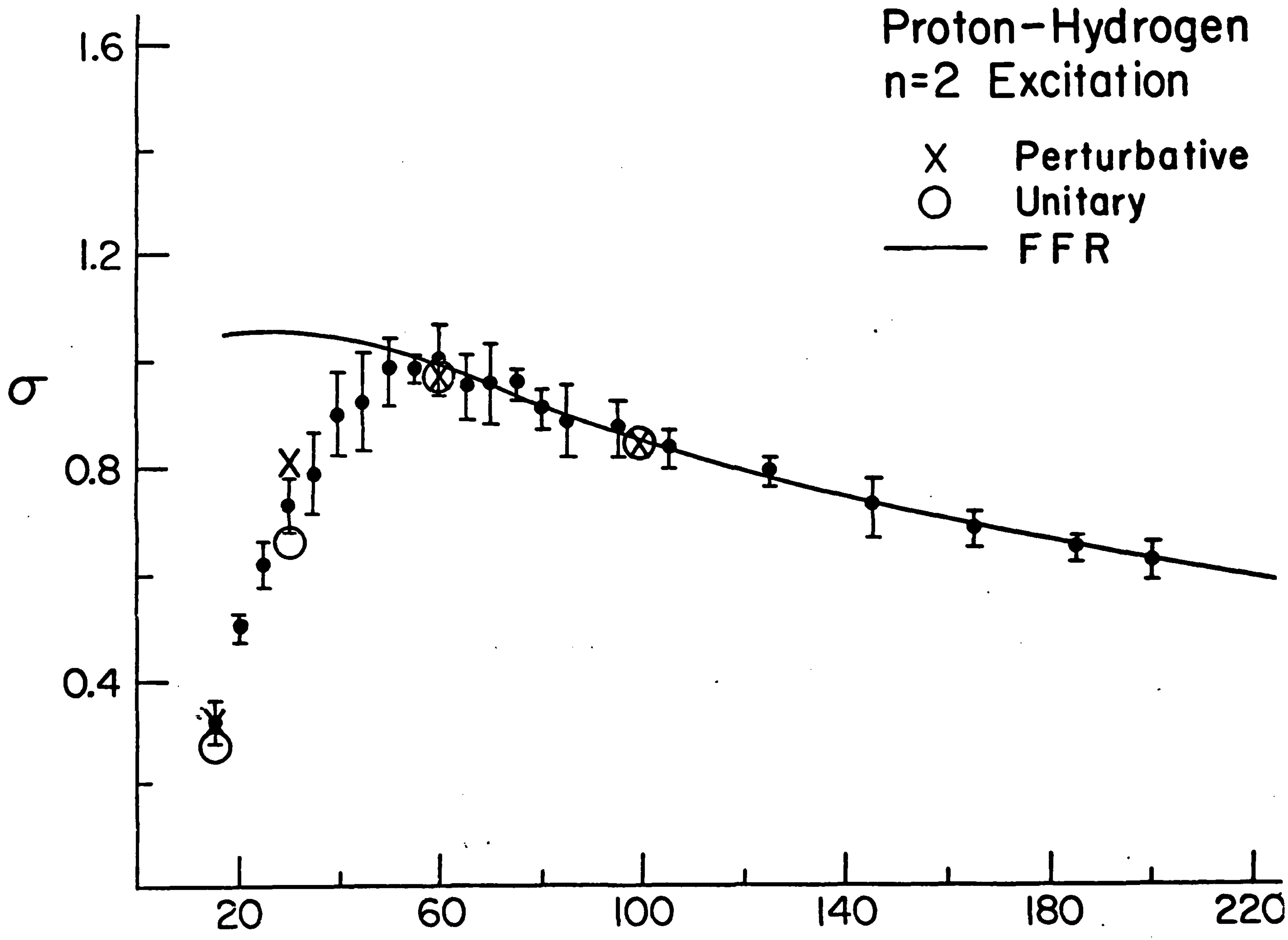
We are of course continuing to explore the areas we have talked about in the previous section as new experiments become available. We have also started some new lines of inquiry. Negatively charged projectiles such as antiprotons, muons, pions, and even electrons

Figure Captions for figs. 6-8

Figure 6. Cross section (in units of $10^{-16} cm^2$) for n=2 excitation in proton-hydrogen collisions. The experimental points (with error bars) are from Park et al (1975 and 1976). The solid curve is our theoretical single-centered expansion result, and is very similar to that published previously (Fitchard et al 1977). The crosses and open circles are results from the perturbative and unitary OHCE methods, respectively, that are described in the text.

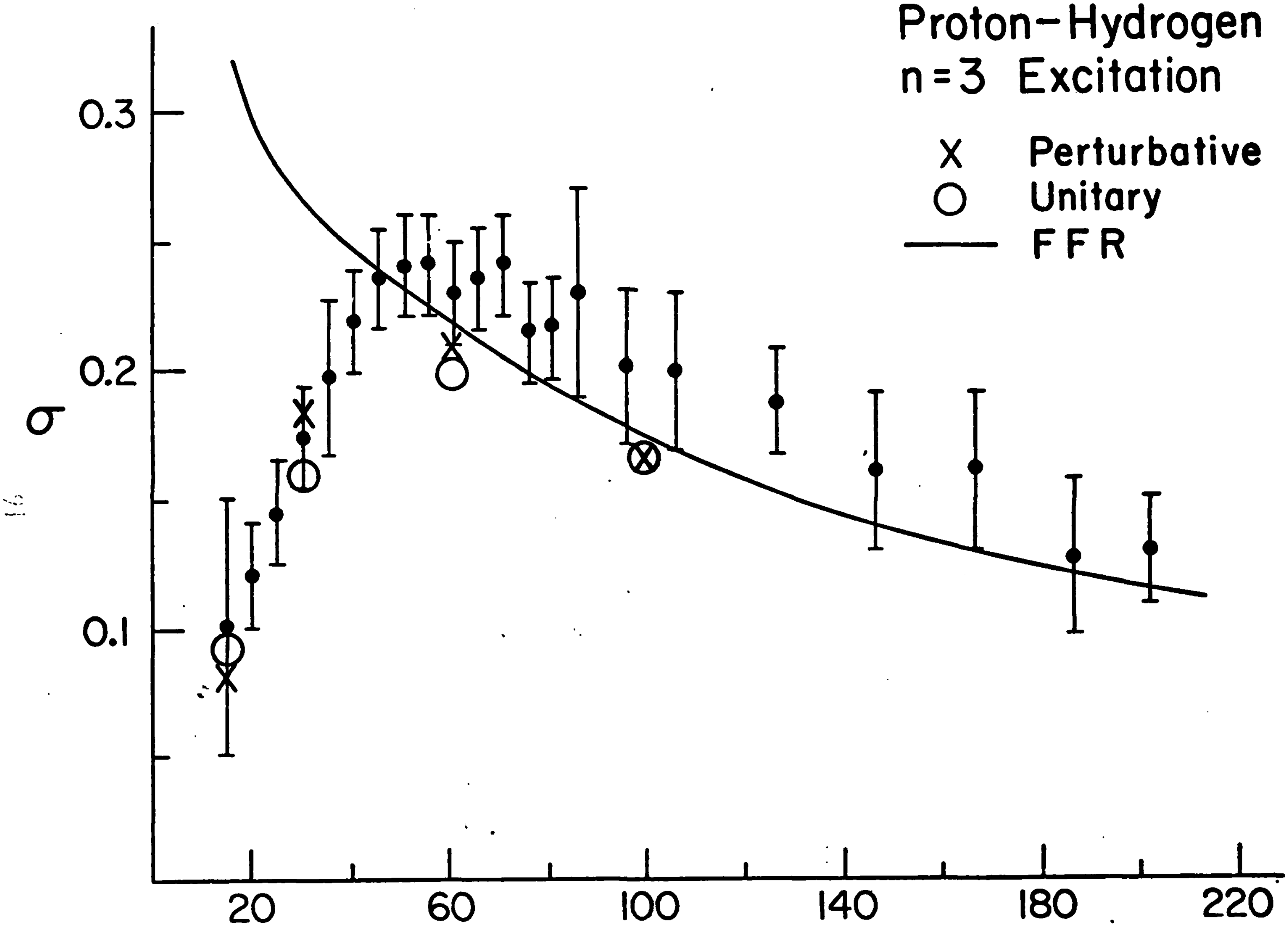
Figure 7. Cross section (in units of $10^{-16} cm^2$) for n=3 excitation in proton-hydrogen collisions. The points and curve are as in figure 1.

Figure 8. Cross section (in units of $10^{-15} cm^2$) for ionisation in proton-hydrogen collisions. The solid curve, crosses, and open circles are the results of our single centered expansion, perturbative OHCE, and unitary OHCE calculations, respectively, as in figures 1 and 2. The experimental points (with error bars) are from the following sources: triangles, Park et al (1977); squares, Fite et al (1960); circles, Gilbody and Ireland (1963).



Proton-Hydrogen
n=2 Excitation
X Perturbative
O Unitary
FFR
1.6
1.2
0.8
0.4
σ
20
60
100
140
180
220
Energy (keV)

Fig. 6.



Proton-Hydrogen
n=3 Excitation
X Perturbative
O Unitary
FFR
0.3
0.2
0.1
σ
20
60
100
140
180
220
Energy (keV)

Fig. 7.

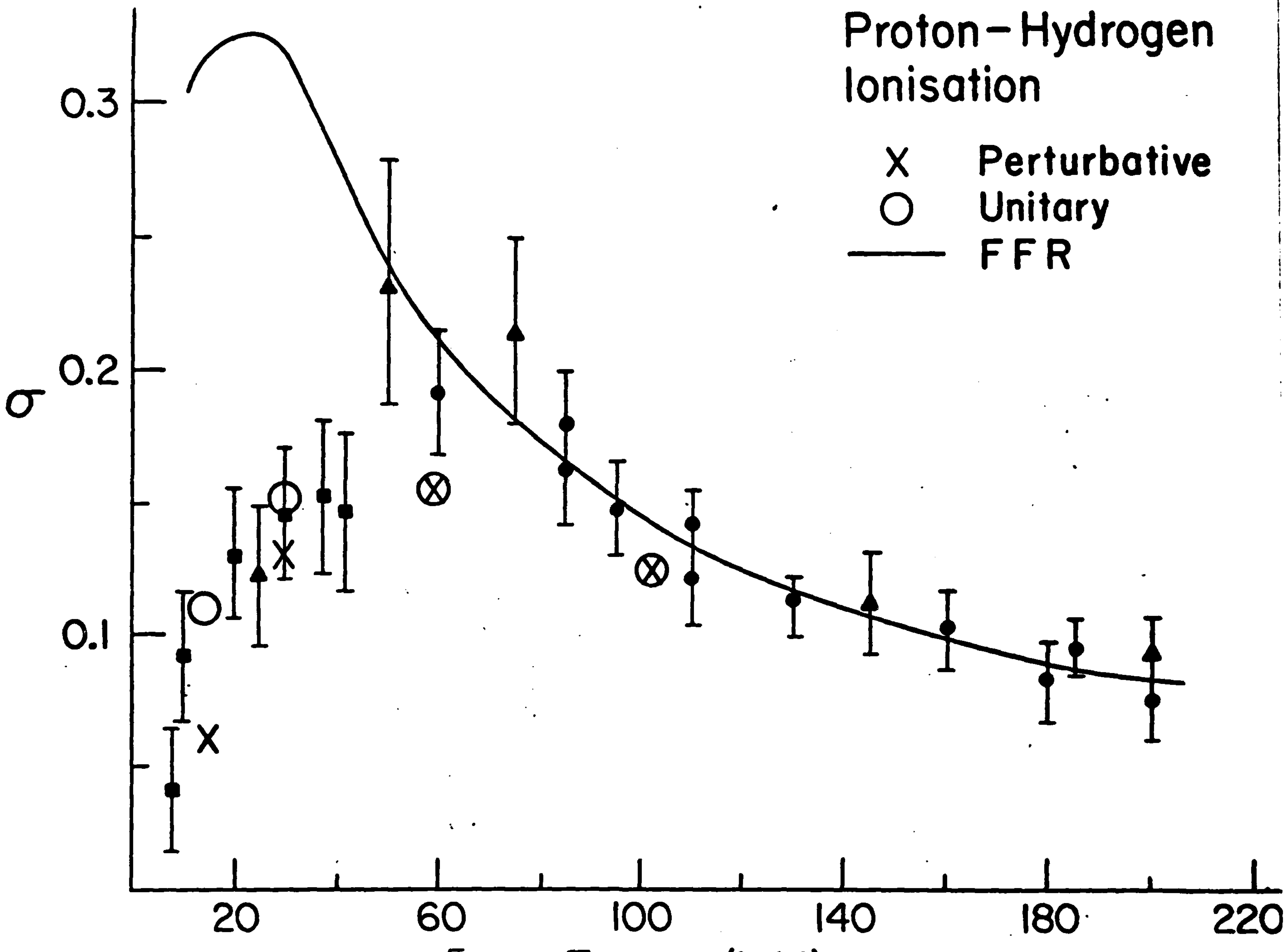

Proton-Hydrogen
Ionisation
X Perturbative
O Unitary
FFR
0.3
0.2
0.1
σ
20
60
100
140
180
220
Energy (keV)

Fig. 8.

can be treated by our code. Charge transfer is not present for these projectiles, and the comparison between cross sections for projectiles of opposite charges should prove interesting. L-shell direct ionization and charge transfer is another topic we have started to explore. This demanded an increase in the number of ℓ-values kept by our code. We have now rewritten the ionization code so that the number of ℓ-values kept is perfectly general, and some L-shell ionization calculations have been carried out. Another important area we are studying is the impact parameter dependence of ionization and of charge transfer, which can be measured experimentally as differential (in projectile scattering angle) cross sections. Finally, we are working on new methods for calculating exchange matrix elements. Our aim here is to improve the efficiency of our codes, to allow for more partial waves to be included, and to allow for more projectile-centered functions to be included in the expansion of eq. (5).

APPENDIX

This appendix gives the abstracts of papers and talks based on work carried out under this contract.

1. (Published in Journal of Physics B 13, 4059 (1980).)

CONTRIBUTIONS OF MULTI-ELECTRON PROCESSES TO INNER-SHELL CHARGE TRANSFER AND VACANCY PRODUCTION: PROJECTILE CHARGE DEPENDENCE IN COLLISIONS OF BARE NUCLEI WITH ARGON

R. L. Becker, A. L. Ford and J. F. Reading

Physics Division, Oak Ridge National Laboratory. Oak Ridge, Tn 37830, USA
Cyclotron Institute and Physics Department, Texas A&M University, College Station, Tx 77843, USA

ABSTRACT. Previous coupled-channels calculations of inner-shell charge transfer and vacancy production for p + Ar collisions are extended to bare projectiles with nuclear charges $Z_p = 2$ and 6, in the collision energy range from 1 to 9 MeV/amu. An improved expression for the charge transfer amplitude is derived in a 'distorted-phase' formulation of the impact parameter method. It provides a better treatment of the contributions from the long-range parts of the interaction potentials. We denote by $\sigma_{C,VK}$ the inclusive cross section, which has been measured by coincidence experiments, for producing all final states in which at least one target electron has been transferred to the projectile and at least one vacancy has been produced in the target K shell. In the single-particle model $\sigma_{C,VK}$ reduces to $\sigma^{SP}_{C,VK}$, which contains only the exclusive single-electron process of direct transfer from the target K shell. In the independent particle model, in which the closed-shells target ground state is represented by a single Slater determinant, multi-electron processes, such as transfer from the L shell, together with ionisation or excitation from the K shell, contribute to $\sigma_{C,VK}$. Different pathways (reaction mechanisms) leading to the same final state have interfering amplitudes.

For example, there is interference between transfer from the K shell and transfer from the L shell accompanied by excitation from the K shell to fill the hole in the L shell (the Pauli exclusion principle forbids excitation to any other L shell substate).

The contributions of multi-electron processes to our calculated $\sigma^{IPM}_{C,VK}$ increase strongly with Z_p. For $Z_p = 6$, $\sigma^{IPM}_{C,VK}$ differs by up to a factor of three from $\sigma^{SP}_{C,VK}$. The present results are combined with the p+ Ar results of a previous paper to give the projectile nuclear charge dependence of $\sigma^{IPM}_{C,VK}$, of the total charge transfer cross section, σ^{IPM}_{CT}, of the total K shell vacancy cross section, σ^{IPM}_{VK}, and of the single-particle approximation to the inclusive ionisation (K shell vacancy) cross section, $\sigma^{SP}_{I,VK}$. The charge transfer cross sections σ^{IPM}_{CT} and $\sigma^{IPM}_{C,VK}$ show a Z_p dependence less than the Z_p^5 of the OBK approximation, in quantitative agreement with the experiments of Rodbro and co-workers with neon targets. The calculated σ^{IPM}_{VK} and $\sigma^{SP}_{I,VK}$ for $Z_p = 6$ are compared with experimental K vacancy production cross sections for C^{6+} and C^{4+} projectiles, respectively, and good agreement is found.

Research participant, summer 1979, Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA.

Research sponsored by the Division of Basic Energy Sciences, US Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.

Research sponsored by the Office of Naval Research, and by the Center for Energy and Mineral Resources, Texas A&M University.

2. (Accepted for publication in Phys. Rev. A).

Inner-Shell Capture and Ionization in Collisions of H^+, He^{2+}, and Li^{3+} Projectiles with Neon and Carbon

A. L. Ford* and J. F. Reading*

Physics Department, Texas A&M University, College Station, Texas 77843

R. L. Becker

Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

Theoretical methods used previously for H^+, He^{2+}, and C^{6+} collisions with neutral argon atoms have been applied to collisions of H^+, He^{2+}, and Li^{3+} projectiles with neon, and to collisions of H^+ with carbon targets. The energy range covered by the calculations is 0.4 to 4.0 MeV/amu for the neon target, and 0.2 to 2.0 MeV/amu for carbon. We calculate single-electron amplitudes for target K-shell ionization and target K-and L-shell, to projectile K-shell, charge transfer. These single-electron amplitudes are used, in an independent particle model that allows for multi-electron processes, to compute K-shell vacancy production cross sections $\sigma^{IPM}_{C,VK}$ for producing a charge transfer state of the projectile in coincidence with a K-shell vacancy in the target. These cross sections are in reasonable agreement with the recent experiments of Rodbro et al. at Aarhus. In particular, the calculated, as well as the experimental, $\sigma_{C,VK}$ scale with projectile nuclear charge Z_p less strongly than the Z_p^5 of the OBK approximation. For He^{2+} and Li^{3+} projectiles at collision energies below where experimental data is available, our calculated multi-electron corrections to the single electron approximation for $\sigma_{C,VK}$ are large.

*Research Participants, Summer 1979, Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830.

Research sponsored at Texas A&M by the U. S. National Science Foundation, the U. S. office of Naval Research and the Center for Energy and Mineral Resources at Texas A&M University.
Research sponsored at ORNL by Division of Basic Energy Sciences, U. S. Department of Energy under contract W-7405-eng-26 Union Carbide Corp.
*Summer research participant Oak Ridge National Laboratory, 1979.

3. (Submitted for publication to Journal of Physics B, and presented at the X80 Conference, Stirling, Scotland, 1980.)

A new atomic orbital method for ion atom collisions

J. F. Reading *, A. L. Ford * and R. L. Becker

Department of Physics, Texas A&M University,
College Station, TX 77843, USA

Physics Division, Oak Ridge National Laboratory,
Oak Ridge, TN 37830, USA

In a series of recent papers we have studied the inner shell direct ionization and charge transfer processes that occur when a light ion, nuclear charge Z_p, collides with a target atom, nuclear charge Z_T. We used a single centered expansion (SCE) method expanding the single electron wave functions in a set of target centered Hilbert states. This method is inaccurate if charge transfer is an important channel for electron flux loss and is thus generally restricted to the asymmetric region, $Z_p \ll Z_T$, in its range of applicability. In this paper we present a new atomic orbital method which allows for charge transfer through prechosen time dependent amplitudes which equal the "real" amplitudes only at large times. The target excitation and ionization amplitudes are found variationally but constrained to produce consistent charge transfer amplitudes. The method has the computational efficiency of an SCE approach. We show in an application to the proton hydrogen problem that it removes the known difficulties that the SCE method had for this symmetric collision. It is hoped that this inexpensive method will find general application to ion-atom collisions in that region of energy where the atomic orbital method is useful.

Acknowledgments

This research was supported at Texas A&M by the Office of Naval Research and by the Center for Energy and Mineral Resources, Texas A&M University. At Oak Ridge the research was sponsored by the Division of Basic Energy Sciences, U. S. Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.

4. (Presented at the 6th Conference on the Application of Accelerators in Research and Industry, Denton, Texas, 1980. Will be published in IEEE Transactions on Nuclear Science, Vol. N528, April, 1981.)

L-SHELL IONIZATION IN PROTON AND ALPHA PARTICLE COLLISIONS WITH ARGON

A. F. Ford, M. Martir, and J. F. Reading

Department of Physics
Texas A&M University, College Station, Texas 77843

SUMMARY

We report results of coupled-state calculations of argon L-shell ionization by proton and alpha particle collisions in the 100 to 500 kev/amu energy range. Our target-centered basis includes up through f-states. We have explored the angular momentum convergence and ability of our pseudostates to describe the ionization continuum by comparing to the Born calculations of Choi; excellent agreement is obtained. In the Born we have shown the effect of using different independent-particle target potentials; these effects are large, particularly at low energy. We propose a modification of the Hartree-Fock potential that leaves all the wavefunctions and the bound orbital energies unaltered, but that lowers the continuum by an amount that brings the L-shell ionization potentials roughly into agreement with experiment. Our coupled-states calculations show deviations from the 1st Born approximation, and are in fair agreement with experiment. A complete comparison to experiment will require the calculation of the charge transfer channel contribution to the vacancy production.

ACKNOWLEDGMENTS

These calculations were supported by the Office of Naval Research, the National Science Foundation, and the Center for Energy and Mineral Resources at Texas A&M.